

Sebacic acid, isoheptyl 4-isopropoxyphenyl ester

Inchi:	InChI=1S/C25H40O5/c1-20(2)12-11-19-28-24(26)13-9-7-5-6-8-10-14-25(27)30-23-17-15
InchiKey:	DWAMIJYOOCLZRG-UHFFFAOYSA-N
Formula:	C25H40O5
SMILES:	CC(C)CCCOC(=O)CCCCCCCC(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]:	420.58

Physical Properties

Property code	Value	Unit	Source
gf	-315.32	kJ/mol	Joback Method
hf	-966.65	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	94.13	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.479		Crippen Method
mvol	360.100	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	2971.00		NIST Webbook
tb	977.18	K	Joback Method
tc	1196.35	K	Joback Method
tf	547.00	K	Joback Method
vc	1.381	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.69	J/molxK	977.18	Joback Method
cpg	1228.12	J/molxK	1013.71	Joback Method
cpg	1242.90	J/molxK	1050.24	Joback Method
cpg	1256.05	J/molxK	1086.77	Joback Method
cpg	1267.60	J/molxK	1123.29	Joback Method
cpg	1277.58	J/molxK	1159.82	Joback Method
cpg	1286.02	J/molxK	1196.35	Joback Method
dvisc	0.0002896	Paxs	547.00	Joback Method
dvisc	0.0001356	Paxs	618.70	Joback Method

dvisc	0.0000744	Paxs	690.39	Joback Method
dvisc	0.0000456	Paxs	762.09	Joback Method
dvisc	0.0000305	Paxs	833.79	Joback Method
dvisc	0.0000217	Paxs	905.48	Joback Method
dvisc	0.0000162	Paxs	977.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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